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2-[(2-Methylphenyl)amino]quinoline-3-carboxylic acid

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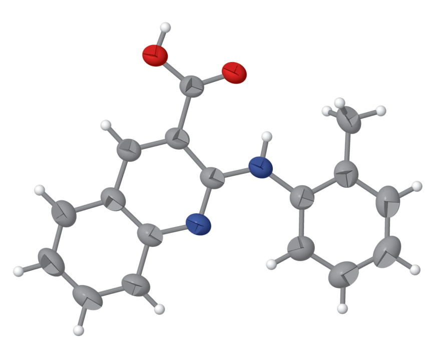
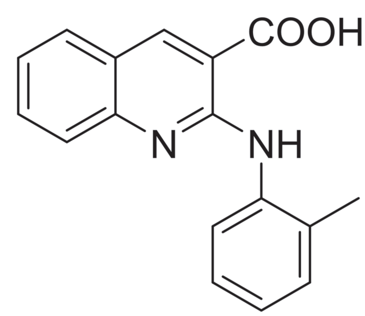
In the title compound, $C_{17}H_{14}N_2O_2$, the dihedral angle between the quinoline ring system and the pendant phenyl ring is 6.19 (6)° and an intramolecular N—H···O hydrogen bond supports the near-planar conformation. In the extended structure, the molecules associate to form centrosymmetric carboxylic acid dimers linked by pairs of O—H···O hydrogen bonds.

3D view



Chemical scheme



Structure description

Nonsteroidal anti-inflammatory drugs (NSAIDs) are a class of drugs that do not contain a steroidal structure but possess anti-inflammatory, analgesic, and antipyretic effects (Ho *et al.*, 2018). NSAIDs mainly exert their anti-inflammatory and analgesic effects by inhibiting cyclooxygenase (COX), thereby reducing the production of prostaglandins. Salicylic acid was the first NSAID to be discovered (Jiang *et al.*, 2018). Following salicylic acid, benzoic acid and nicotinic acid derivatives became important NSAIDs, exemplified by tolfenamic acid and clonixin. These anti-inflammatory drugs have been found to exhibit polymorphism. For example, tolfenamic acid has been found to have nine crystal forms (Subaiea *et al.*, 2011). As part of our studies in this area, we now describe the synthesis and structure of the title compound, $C_{17}H_{14}N_2O_2$ (**I**).

Compound (**I**) (Fig. 1) is an analogue of 2-(phenylamino)nicotinic acid (Long *et al.*, 2008), which is a compound with rich polymorphism. In the new compound, a quinoline ring replaces the pyridine ring. The C1–C9/N1 quinoline and pendant C10–C15 phenyl rings are almost coplanar, with a dihedral angle of 6.19 (6)° and an intramolecular N—H···O hydrogen bond (Table 1) supports the near-planar conformation. In the extended structure, the molecules associate to form centrosymmetric carboxylic-acid dimers linked by pairs of O—H···O hydrogen bonds (Fig. 2).

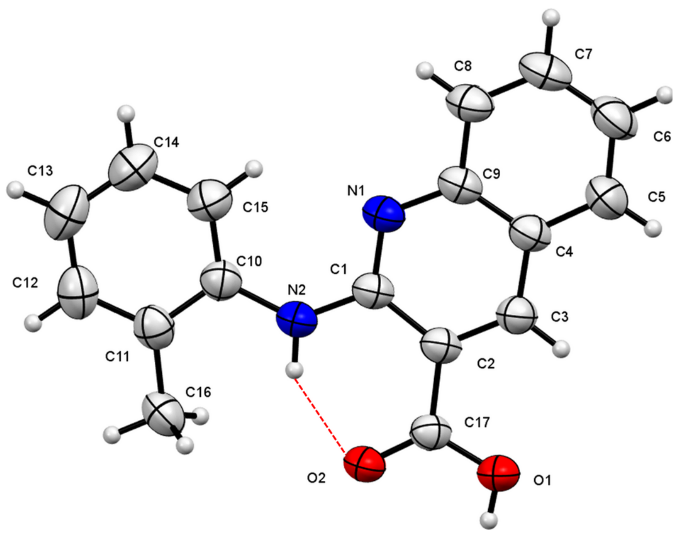


Figure 1
The molecular structure of (**I**) drawn at the 50% probability level. The intramolecular hydrogen bond is shown as a dashed line.

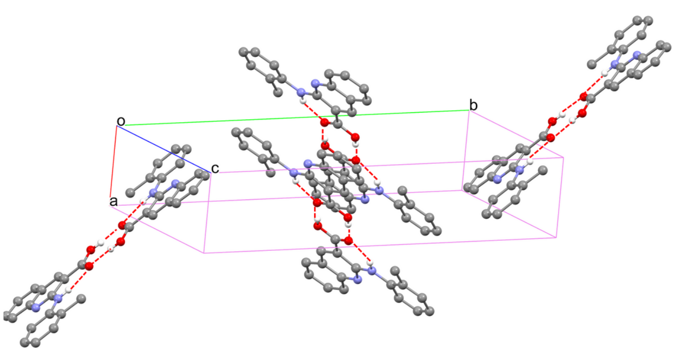


Figure 2
Packing of the molecules in (**I**) with hydrogen bonds shown as red dashed lines (for clarity, H atoms not involved in hydrogen bonding are omitted).

Synthesis and crystallization

The title compound was synthesized in two steps using a Buchwald–Hartwig cross-coupling reaction and a hydrolysis reaction (Fig. 3). The compound was purified by column chromatography. Single crystals in the form of yellow needles were obtained by slowly evaporating an acetone solution of the title compound.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

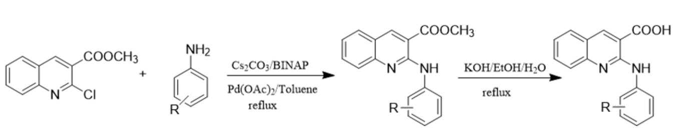


Figure 3
Synthesis scheme for (**I**).

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···O2	0.86	1.97	2.6956 (14)	141
O1—H1···O2^{i}	0.82	1.85	2.6684 (13)	177

Symmetry code: (i) $-x+2, -y+1, -z+1$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{17}H_{14}N_2O_2$
M_r	278.30
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	300
a, b, c (Å)	4.9122 (1), 24.0804 (6), 11.5773 (2)
β (°)	90.220 (2)
V (Å^3)	1369.44 (5)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	0.73
Crystal size (mm)	0.2 × 0.08 × 0.07
Data collection	
Diffractometer	ROD, Synergy Custom system, HyPix
Absorption correction	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2024)
T_{min}, T_{max}	0.606, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	11254, 2830, 2380
R_{int}	0.032
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.633
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.040, 0.121, 1.06
No. of reflections	2830
No. of parameters	193
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.19, −0.14

Computer programs: *CrysAlis PRO* (Rigaku OD, 2024), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2018/3* (Sheldrick, 2015*b*) a *OLEX2* (Dolomanov *et al.*, 2009).

Acknowledgements

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References

Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). *J. Appl. Cryst.* **42**, 339–341.
Ho, K. Y., Gwee, K. A., Cheng, Y. K., Yoon, K. H., Heen, H. T. & Omar, A. R. (2018). *J. Pain Res.* **11**, 1937–1948.
Jiang, W. S., Wang, L. G., Zhang, J. G., Shen, H. C., Dong, W., Zhang, T. H., Li, X. W., Wang, K. & Du, J. J. (2018). *Medicine* **97**, e12442.
Long, S. H., Parkin, S., Siegler, M. A., Cammers, A. & Li, T. L. (2008). *Cryst. Growth Des.* **8**, 4006–4013.
Rigaku OD (2024). *CrysAlis PRO*. Rigaku Oxford Diffraction, Yarnton, England.
Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.
Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.
Subaiea, G. M., Alansi, B. H., Serra, D. A., Alwan, M. & Zawia, N. H. (2011). *Curr. Alzheimer Res.* **8**, 860–867.

full crystallographic data

IUCrData (2026). **11**, x260554 [https://doi.org/10.1107/S2414314626005547]

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Crystal data

$C_{17}H_{14}N_2O_2$
M_r = 278.30
Monoclinic, $P2_1/n$
a = 4.9122 (1) Å
b = 24.0804 (6) Å
c = 11.5773 (2) Å
β = 90.220 (2)°
V = 1369.44 (5) Å^3
Z = 4
F(000) = 584
D_x = 1.350 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54184 Å
Cell parameters from 6020 reflections
θ = 3.7–77.1°
μ = 0.73 mm^{-1}
T = 300 K
Needle, clear dark yellow
0.2 × 0.08 × 0.07 mm

Data collection

ROD, Synergy Custom system, HyPix diffractometer
Radiation source: Rotating-anode X-ray tube, Rigaku (Cu) X-ray Source
Mirror monochromator
Detector resolution: 10.0000 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlisPro; Rigaku OD, 2024)
T_{min} = 0.606, T_{max} = 1.000
11254 measured reflections
2830 independent reflections
2380 reflections with $I > 2\sigma(I)$
R_{int} = 0.032
θ_{max} = 77.6°, θ_{min} = 3.7°
h = −5→6
k = −30→30
l = −14→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.121
S = 1.06
2830 reflections
193 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0605P)^2 + 0.1663P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ < 0.001
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}
Extinction correction: SHELXL2018/3 (Sheldrick 2015b), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0043 (8)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. The H atoms were placed in idealized locations and refined as riding atoms.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.86071 (19)	0.50007 (4)	0.64825 (8)	0.0544 (3)
H1	0.972645	0.514724	0.605628	0.082*
O2	0.76184 (18)	0.45416 (4)	0.48683 (8)	0.0528 (3)
N1	0.1504 (2)	0.36553 (5)	0.67276 (10)	0.0489 (3)
N2	0.3664 (2)	0.37672 (5)	0.49696 (10)	0.0514 (3)
H2	0.493564	0.394442	0.461808	0.062*
C1	0.3361 (2)	0.39115 (5)	0.60958 (11)	0.0434 (3)
C2	0.5062 (2)	0.43478 (5)	0.65729 (10)	0.0427 (3)
C3	0.4650 (3)	0.44993 (6)	0.76930 (11)	0.0487 (3)
H3	0.571032	0.478019	0.801326	0.058*
C4	0.2651 (3)	0.42393 (6)	0.83770 (11)	0.0485 (3)
C5	0.2115 (3)	0.43787 (8)	0.95348 (13)	0.0656 (4)
H5	0.306527	0.466831	0.988248	0.079*
C6	0.0207 (3)	0.40921 (8)	1.01528 (13)	0.0688 (4)
H6	−0.013247	0.418603	1.091801	0.083*
C7	−0.1219 (3)	0.36607 (7)	0.96347 (14)	0.0636 (4)
H7	−0.249664	0.346493	1.006340	0.076*
C8	−0.0788 (3)	0.35180 (6)	0.85132 (13)	0.0569 (4)
H8	−0.177882	0.322935	0.818292	0.068*
C9	0.1164 (2)	0.38075 (5)	0.78466 (11)	0.0461 (3)
C10	0.2272 (3)	0.33793 (6)	0.42729 (12)	0.0493 (3)
C11	0.2962 (3)	0.33752 (6)	0.31000 (12)	0.0520 (3)
C12	0.1663 (3)	0.29969 (7)	0.23774 (14)	0.0630 (4)
H12	0.212688	0.298684	0.159966	0.076*
C13	−0.0303 (4)	0.26344 (7)	0.27837 (17)	0.0706 (5)
H13	−0.116345	0.238710	0.228478	0.085*
C14	−0.0961 (4)	0.26463 (7)	0.39330 (17)	0.0692 (4)
H14	−0.228135	0.240482	0.421178	0.083*
C15	0.0303 (3)	0.30104 (7)	0.46839 (14)	0.0619 (4)
H15	−0.015566	0.301025	0.546256	0.074*
C16	0.5042 (3)	0.37707 (7)	0.26173 (13)	0.0626 (4)
H16A	0.450583	0.414562	0.278322	0.094*
H16B	0.516342	0.372110	0.179635	0.094*
H16C	0.678339	0.369766	0.296465	0.094*
C17	0.7195 (2)	0.46328 (5)	0.58959 (11)	0.0432 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0490 (5)	0.0645 (6)	0.0498 (5)	−0.0156 (4)	0.0073 (4)	−0.0006 (4)
O2	0.0487 (5)	0.0648 (6)	0.0449 (5)	−0.0131 (4)	0.0084 (4)	0.0016 (4)
N1	0.0468 (6)	0.0531 (6)	0.0468 (6)	−0.0057 (5)	0.0081 (4)	0.0046 (5)
N2	0.0487 (6)	0.0606 (7)	0.0450 (6)	−0.0125 (5)	0.0084 (5)	−0.0009 (5)
C1	0.0383 (6)	0.0480 (6)	0.0439 (6)	0.0002 (5)	0.0035 (5)	0.0063 (5)
C2	0.0363 (6)	0.0493 (7)	0.0426 (6)	0.0002 (5)	0.0024 (5)	0.0065 (5)

C3	0.0444 (6)	0.0566 (7)	0.0450 (7)	−0.0059 (5)	0.0017 (5)	0.0022 (6)
C4	0.0438 (6)	0.0587 (8)	0.0430 (6)	0.0003 (5)	0.0047 (5)	0.0062 (5)
C5	0.0653 (9)	0.0845 (11)	0.0470 (8)	−0.0111 (8)	0.0093 (6)	−0.0048 (7)
C6	0.0693 (9)	0.0914 (12)	0.0458 (8)	−0.0020 (9)	0.0164 (7)	0.0040 (8)
C7	0.0584 (8)	0.0751 (10)	0.0576 (8)	−0.0008 (7)	0.0194 (7)	0.0149 (8)
C8	0.0542 (7)	0.0584 (8)	0.0584 (8)	−0.0066 (6)	0.0134 (6)	0.0084 (6)
C9	0.0420 (6)	0.0505 (7)	0.0460 (6)	0.0039 (5)	0.0063 (5)	0.0079 (5)
C10	0.0457 (6)	0.0515 (7)	0.0507 (7)	0.0004 (5)	0.0007 (5)	−0.0024 (6)
C11	0.0498 (7)	0.0555 (7)	0.0506 (7)	0.0092 (6)	0.0005 (5)	−0.0038 (6)
C12	0.0714 (9)	0.0627 (9)	0.0550 (8)	0.0123 (7)	−0.0063 (7)	−0.0105 (7)
C13	0.0747 (10)	0.0566 (9)	0.0803 (12)	0.0010 (7)	−0.0198 (9)	−0.0141 (8)
C14	0.0666 (9)	0.0608 (9)	0.0802 (11)	−0.0133 (7)	−0.0060 (8)	−0.0029 (8)
C15	0.0618 (8)	0.0632 (9)	0.0606 (9)	−0.0130 (7)	0.0022 (7)	−0.0012 (7)
C16	0.0662 (9)	0.0747 (10)	0.0470 (7)	0.0003 (7)	0.0132 (6)	−0.0026 (7)
C17	0.0371 (6)	0.0488 (7)	0.0437 (6)	−0.0009 (5)	0.0000 (5)	0.0053 (5)

Geometric parameters (Å, º)

O1—H1	0.8200	C7—H7	0.9300
O1—C17	1.3129 (16)	C7—C8	1.360 (2)
O2—C17	1.2284 (15)	C8—H8	0.9300
N1—C1	1.3239 (15)	C8—C9	1.4164 (17)
N1—C9	1.3573 (17)	C10—C11	1.4008 (19)
N2—H2	0.8600	C10—C15	1.398 (2)
N2—C1	1.3582 (17)	C11—C12	1.390 (2)
N2—C10	1.4096 (18)	C11—C16	1.506 (2)
C1—C2	1.4503 (18)	C12—H12	0.9300
C2—C3	1.3629 (18)	C12—C13	1.385 (3)
C2—C17	1.4797 (16)	C13—H13	0.9300
C3—H3	0.9300	C13—C14	1.371 (3)
C3—C4	1.4105 (18)	C14—H14	0.9300
C4—C5	1.408 (2)	C14—C15	1.380 (2)
C4—C9	1.410 (2)	C15—H15	0.9300
C5—H5	0.9300	C16—H16A	0.9600
C5—C6	1.368 (2)	C16—H16B	0.9600
C6—H6	0.9300	C16—H16C	0.9600
C6—C7	1.388 (3)		
C17—O1—H1	109.5	N1—C9—C8	118.25 (13)
C1—N1—C9	119.29 (12)	C4—C9—C8	118.43 (12)
C1—N2—H2	114.2	C11—C10—N2	116.15 (12)
C1—N2—C10	131.61 (11)	C15—C10—N2	124.14 (13)
C10—N2—H2	114.2	C15—C10—C11	119.72 (13)
N1—C1—N2	119.31 (12)	C10—C11—C16	121.48 (13)
N1—C1—C2	121.62 (12)	C12—C11—C10	118.41 (14)
N2—C1—C2	119.07 (11)	C12—C11—C16	120.11 (13)
C1—C2—C17	122.84 (11)	C11—C12—H12	119.1
C3—C2—C1	117.96 (11)	C13—C12—C11	121.83 (15)

C3—C2—C17	119.20 (12)	C13—C12—H12	119.1
C2—C3—H3	119.3	C12—C13—H13	120.5
C2—C3—C4	121.44 (13)	C14—C13—C12	118.91 (15)
C4—C3—H3	119.3	C14—C13—H13	120.5
C5—C4—C3	124.19 (14)	C13—C14—H14	119.4
C5—C4—C9	119.48 (12)	C13—C14—C15	121.18 (16)
C9—C4—C3	116.33 (12)	C15—C14—H14	119.4
C4—C5—H5	119.7	C10—C15—H15	120.0
C6—C5—C4	120.58 (16)	C14—C15—C10	119.94 (15)
C6—C5—H5	119.7	C14—C15—H15	120.0
C5—C6—H6	120.1	C11—C16—H16A	109.5
C5—C6—C7	119.81 (15)	C11—C16—H16B	109.5
C7—C6—H6	120.1	C11—C16—H16C	109.5
C6—C7—H7	119.3	H16A—C16—H16B	109.5
C8—C7—C6	121.42 (14)	H16A—C16—H16C	109.5
C8—C7—H7	119.3	H16B—C16—H16C	109.5
C7—C8—H8	119.9	O1—C17—C2	114.38 (11)
C7—C8—C9	120.26 (15)	O2—C17—O1	122.04 (11)
C9—C8—H8	119.9	O2—C17—C2	123.57 (11)
N1—C9—C4	123.31 (11)		

N1—C1—C2—C3	−1.65 (19)	C4—C5—C6—C7	−0.2 (3)
N1—C1—C2—C17	178.61 (11)	C5—C4—C9—N1	178.35 (13)
N2—C1—C2—C3	177.62 (12)	C5—C4—C9—C8	−1.5 (2)
N2—C1—C2—C17	−2.12 (18)	C5—C6—C7—C8	−0.8 (3)
N2—C10—C11—C12	179.45 (13)	C6—C7—C8—C9	0.5 (2)
N2—C10—C11—C16	−1.0 (2)	C7—C8—C9—N1	−179.25 (14)
N2—C10—C15—C14	179.76 (15)	C7—C8—C9—C4	0.6 (2)
C1—N1—C9—C4	1.7 (2)	C9—N1—C1—N2	−178.68 (12)
C1—N1—C9—C8	−178.45 (12)	C9—N1—C1—C2	0.59 (19)
C1—N2—C10—C11	174.13 (13)	C9—C4—C5—C6	1.3 (2)
C1—N2—C10—C15	−6.0 (2)	C10—N2—C1—N1	1.6 (2)
C1—C2—C3—C4	0.49 (19)	C10—N2—C1—C2	−177.73 (13)
C1—C2—C17—O1	−177.35 (11)	C10—C11—C12—C13	1.0 (2)
C1—C2—C17—O2	3.29 (19)	C11—C10—C15—C14	−0.3 (2)
C2—C3—C4—C5	−179.58 (14)	C11—C12—C13—C14	−0.7 (2)
C2—C3—C4—C9	1.5 (2)	C12—C13—C14—C15	−0.1 (3)
C3—C2—C17—O1	2.91 (17)	C13—C14—C15—C10	0.6 (3)
C3—C2—C17—O2	−176.45 (12)	C15—C10—C11—C12	−0.5 (2)
C3—C4—C5—C6	−177.53 (15)	C15—C10—C11—C16	179.12 (14)
C3—C4—C9—N1	−2.7 (2)	C16—C11—C12—C13	−178.60 (15)
C3—C4—C9—C8	177.40 (12)	C17—C2—C3—C4	−179.76 (12)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O2	0.86	1.97	2.6956 (14)	141

O1—H1···O2^{i}	0.82	1.85	2.6684 (13)	177

Symmetry code: (i) −*x*+2, −*y*+1, −*z*+1.